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A METHOD FOR SCALING BIOLOGICAL RESPONSE OF SOIL MICROCOSMS

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ABSTRACT

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An extensive series of laboratory experiments was conducted in soil microcosms to study the respiratory response of microorganisms to toxicant amendments within different types of soils. Our analysis of test results demonstrates that coupled biological and environmental factors within soil can be scaled (i.e., commensurably and analogously grouped) by means of two rate constants, one characterizing the diffusion of CO_2 in the soil matrix and another the biological production of CO_2. The two rate constants were used to classify the impact of metal compounds on diverse soil types and to predict the loss or gain of total respiratory CO_2 of amended soils relative to intact soils. This method exemplifies a more general approach, potentially useful for scaling complex physical and biological interactions in environmental assessments.

INTRODUCTION

An assessment of the fate and effects of hazardous substances in the terrestrial environment requires testing in representative soils of diverse biogeochemical characteristics. One approach has been to develop soil model ecosystems (Draggan, 1976; Gillett and Witt, 1979). These simple systems can be used to produce a data base representing diverse soil types. The utility of such data for environmental impact assessment can be greatly enhanced if they are condensed in a manner that: (a) preserves and emphasizes the primary outcome of the experiments; (b) conveniently classifies the results for identification and use; and (c) facilitates their extension to soil systems not actually tested.

Sometimes the above objectives can be realized by using statistical methods like factor analysis, principal component analysis, discriminant func-

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tions, etc. (Kruskal and Tanur, 1968). A successful application of the methods should summarize the data in terms of a smaller number of variables (or dimensions) than contained in the original data set. Also, the reduced dimensions, in some sense, would retain approximately the same information as contained in the original data. To achieve this objective, an investigator must exercise considerable judgment in selecting the statistical package, determining the approximation alogarithm, and assessing the adequacy of the outcome relative to the objectives of the experiments. These and other statistical packages may also be used to classify or cluster the data into groups which in some sense share similar attributes. The criteria for similarity may be based on the relative distances among objects as revealed from a graph of data points or from some other geometric and algebraic criteria, depending on the availability of methods and the investigator's judgment. In this manner, data from many experiments may be pieced together to reveal a pattern and to make possible a general statement about the problem as a whole.

We pursue an alternative approach by starting with a simple model of a soil microcosm, use it to explain individual experiments, and provide a convenient procedure for summarization, classification, and extension of results from one group of experiments to similar, untested soils.

Shirazi (1980) reported the feasibility of developing such an alternative from the application of the theory of similarity (Buckingham, 1907; Luikov, 1966) to general classes of terrestrial microcosms. The rationale underlying the approach can be summarized this way. Systems of differential equations can represent general classes of phenomena. Within these, a smaller subset of those phenomena can be identified by similar geometries and boundary conditions. The theory provides rules for constructing the necessary and sufficient number of dimensionless parameters from geometric and physical properties of the system to serve as scalers for groupings of empirical data.

Each scaler is formed from coupling several of the original variables into one number, thereby reducing the dimensionality of the problem. Together, the scalers provide a smaller number of coordinates than the number of original variables. They can be used to summarize the entire information of an experiment. The original variables may have any units of measure, e.g., length, weight, temperature, etc., but the scalers formed from them are unitless (i.e., dimensionless).

It is always possible to interpret each scaler as a cognate descriptor of the experimental process. As such, each scaler is a 'principal component' of the problem. It is derived from a model describing the theory of many groups of similar processes and not directly from the data after an experiment is conducted.

In this paper we demonstrate an application of this principle to sets of

data obtained from closed microcosms (Bond et al., 1976) each containing one of a set of soils with diverse properties, with or without addition of heavy metal salts known to be soil toxicants (Tyler, 1975; Bond et al., 1976; Van Voris et al., 1980).

MICROCOSM ANALYSIS

The total quantity of CO_2 evolved by microbial respiration in soil microcosms represents an integrated measure of biotic and abiotic factors that may be characterized by the rate constants μ and η, respectively. The biotic constant μ for CO_2 production is much like the intrinsic or specific growth rate constant commonly used in population biology (Slobotkin, 1961) and is measured in units of day^{-1} or equivalent. Values of μ are inversely proportional to the rate of processing of organic matter by soil microbes. The abiotic or environmental rate constant η characterizes the diffusion of CO_2 within the soil matrix and may also be measured in units of day^{-1}. Large values of η would be associated with soils within which diffusion is limited, i.e., those that are nonporous, fine grained, deep, and/or highly compacted.

Common experience and the structure of the experiment lead us to assume that carbon dioxide in the experimental systems is generated mainly by microbial respiration. We also assume CO_2 is not necessarily a limiting substance per se, albeit closely linked to one(s) which might be, e.g., O_2 or respiratory enzymes.

Conceptually, the nature of this interaction is not known. However, we explore in an empirical manner the feasibility of coupling the biotic with the abiotic process in the microcosm by the manner the coupling can best explain the data. Mathematically, this is done rather simply by adding a source term to the equation for diffusion of CO_2 in the soil. The source term represents the biological production of CO_2 everywhere in the soil matrix of the microcosm.

The analogy with population biology leads us to assume an exponential curve for the source term, using the rate constant μ as a parameter in the exponent. Further coupling of the source term with the abiotic process is obtained, likewise, by an exponential function using the rate constant η as a parameter in the exponent.

Since the two processes have opposing effects on diffusion of CO_2, the rate constants appear with opposite signs in the source function; hence $\exp[(\eta - \mu)t]$. This means that coupling is accomplished by making the source function dependent on the difference between the two rate constants. (We have tried other functions, but none explained the data as well in the prediction of the overall trend and the goodness of fit in a least squares sense.)

Again, the analogy with population biology leads us to assume that biological CO_2 production is proportional with the number of microbes in the soil. We have not measured the latter directly. Instead, the respiratory CO_2 is measured as a proxy and the proportionality factor for the process as a whole is reflected in our use of the parameters G_0 in the source function; hence, $G(t) = G_0 \exp[(\eta - \mu)t]$, which is eq. 2 in the Appendix. G_0 relates to the initial conditions affecting soil preparation, inoculation, and incubation. Having no other way of estimating G_0 by a direct measurement, its numerical value for each test was evaluated based on the slope of the CO_2 production at zero time (eq. 4, Appendix).

The solutions of the one dimensional diffusion equation used in this paper are well known and are presented in detail in the Appendix. The above discussion of interaction with a biotic component in the system should explain the reason for appearance of the source function $G(t)$ in the diffusion equation and its solution. The general solution of this system is illustrated in Fig. 1. The response patterns of CO_2 production with time are generalized by presenting the dimensionless coordinate N (time, in multiples of μ) versus the dimensionless CO_2 production Q (in units of η/S). Q is the total CO_2 production that is released at the soil surface from the start of the test at $N = 0$ up to an arbitrary time N. It is an integrated value over the entire depth of the soil in the microcosm. Various curves identify the relative

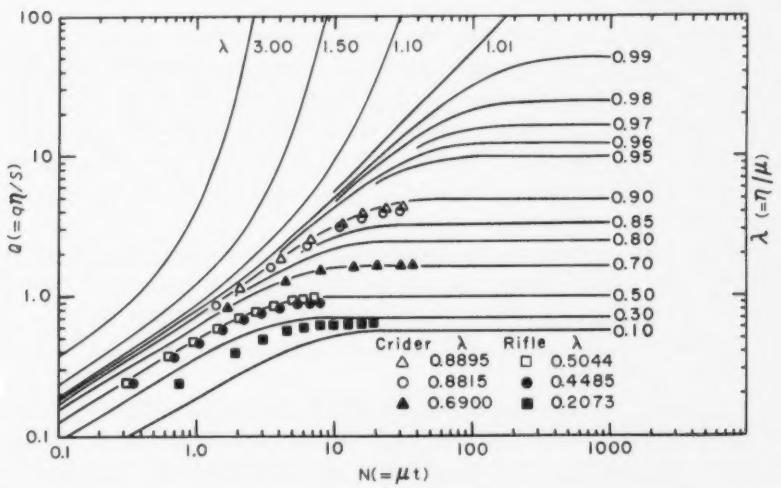

Fig. 1. Theoretical respiratory microcosm response Q expressed in generalized dimensionless coordinates. Data are from Fig. 2. η is diffusion rate constant (day^{-1}), S is the slope of experimental CO_2–time curve at zero time [(mg/g)/day], t is time (day) and q is accumulated CO_2 (mg/g).

ratios (λ) of diffusion to production rate constants. When λ is greater than unity, theoretically there is no biological system limit to CO_2 production. The system is constrained by the ability of O_2 to diffuse into, and CO_2 out of, the soil of that physical and biological structure, to the limit of available carbon. This is a mathematical and graphical illustration of the competition between the biological CO_2 production and the physical resistance to its escape from the soil matrix.

Biological CO_2 production is uniquely characterized by the dimensionless constants N and the rate constant ratio λ. Together, the use of N and λ scale all data for these microcosms, so that any microcosm sharing the same N and λ values should show similar CO_2 production. Analytically, the necessary and sufficient conditions for N and λ to be the scalers of the problem follow directly from the theory and from the general agreement of this theory with the trend in the data. The outcome does not depend upon the absolute magnitudes of other individual soil and biological characteristics, however diverse, entering the calculations of N and λ. Consequently, a wide range of values of N and λ may be sought in practice from a few experiments with soils of known characteristics (i.e., pre-selected porosity, CO_2 diffusivity, and depth). When presented in terms of dimensionless parameters, these empirical results may be extended to other systems not actually tested and having somewhat different soil characteristics, but identical N and λ values. When experiments are extended long enough, the dimensionless total system CO_2 production or, more simply, the 'functional capacity' (Q_∞) of a system becomes dependent solely on λ, so that η and μ are the key parameters for scaling respiration in terrestrial soil systems. We will exploit this theoretical feature to condense our experimental data.

EXPERIMENTAL PROCEDURE

Batches of representative soils (Table I) from the U.S. Soil Conservation Service Soil Repository were air dried and sieved to pass a 2-mm mesh. Soil characteristics, such as porosity, were determined at the conditions of the experiment. Replicate microcosms (Bond et al., 1976) were prepared by placing 100 g of soil into each of three 1-qt [a] jars and adding distilled water and a 1.0-ml inoculum of fresh soil washings to bring the soil to 70% water holding capacity. Aqueous solutions of metal compounds were injected into treated microcosms with a needle system which introduced the solution at 46 locations, giving a predetermined concentration measured in mmole per kg of dry weight soil. In order to restore an acceptable and uniform level of

[a] Liquid quart = $\frac{1}{4}$ USgal = 0.946353 l.

TABLE I

Properties of nine soil series used in microcosm experiment

Soil series (state) properties and classification	Texture [a] < 2 mm		σ_g	Bulk density oven dry (g/ml)	Organic carbon (%)	pH	CEC (meq/100 g	Moisture 70% sat.	Bulk density at 70% sat. (g/ml)	Pore space moist soil, n (%)	Diffusivity of CO_2 [b], α (cm^2/day)	Depth 100 g soil in microcosm, l (cm)	Diffusion rate-constant, $\eta = \alpha/l^2$ (day^{-1})
	Class	d_g (mm)											
"Crider" (KY) fine, silty, mixed, mesic typic Paleudalf	silt	0.0158	7.30	1.17	3.1	6.7	14.0	30	1.07	27	1.36	1.50	0.60
"Dayton" (OR) fine, montmorillonitic, mesic, Albaqualfs	silty clay	0.0152	7.92	1.19	2.6	5.2	12.9	32	1.06	28	1.47	1.50	0.65
"Dixonville" (OR) fine, mixed, mesic Argixerolls	clay	0.0132	13.8	0.92	6.7	5.9	56.7	49	0.81	29	1.57	1.98	0.40
"Jory" (OR) clayey, mixed, mesic Haplohumults	clay	0.0112	14.4	0.91	5.8	6.0	19.3	32	0.81	43	3.46	1.98	0.88

"Rifle" (MI) eudic, typic Borochemist	loam	0.0571	16.5	0.34	64.0	6.2	12.5	172	0.22	47	4.13	7.28	0.078
"Sharpsburg" (WY) Montmorillonitic, mesic typic Argiudoll	sand loam	0.1750	11.2	1.48	1.7	8.1	20.0	23	1.41	14	0.37	1.14	0.28
"Toledo" (OR) fine, illitic, noacid, mesic, mollic Haploquept	clay	0.0102	14.4	1.46	5.5	7.0	25.1	24	1.22	24	1.08	1.32	0.62
"Walla Walla" (WA) coarse, silty, mixed mesic, typic haloxerol	silt loam	0.0286	9.63	1.18	1.7	6.3	18.4	29	1.07	28	1.47	1.50	0.65
"Willamette" (OR) fine, silty, mixed mesic Argixerolls	silty clay	0.0119	8.56	1.06	3.7	4.6	17.7	29	0.94	34	2.16	1.70	0.75

[a] According to USDA convention for soil separate sizes; particle size distributions are shown by two statistics, geometric mean d_g and geometric standard deviation σ_g.
[b] $\alpha = 18.7n^2$. After Buckingham (Baver, 1965).

activity in soils desiccated for varying times in storage, microcosms were inoculated with 1.0 ml of the supernatant (centrifuged at 2000g for 2 min) of a suspension of 100 g of fresh agricultural soil in 1 l of distilled water. Preliminary studies showed that respiration rates were consistent for a given soil after two weeks equilibration, irrespective of the fresh soil source of the inoculum.

The microcosms were maintained in the dark at 20°C for the test duration. Accumulated respiratory CO_2 was measured periodically by the alkali trap/acid titration method (Coleman, 1973). Use of the alkali trap maintains the CO_2 concentration trapped in the air space above the soil in the microcosm jar nearly equal to zero. This boundary condition has been imposed in our analysis of the problem.

It was convenient to conduct the tests for a fixed time, generally 6–8 weeks. The measured respiratory CO_2, P_T, at the end of this period approached the theoretical respiratory capacity Q_∞ to varying degrees but never exactly equaled it.

RESULTS AND ANALYSIS

Several test results typifying patterns of measured CO_2 production are plotted in Fig. 2. These same tests are transformed and plotted in Fig. 1 using identical symbols for each reference. An outline of the procedure for the transformation of a point i belonging to a test j, $(t_i, p_i)_j$, from Fig. 2 to a corresponding point $(N_i, Q_i)_j$ in Fig. 1 is useful for understanding of our results.

Two groups of numbers are needed to effect the transformation; one for the test as a whole and the other for a data point in that test. The group for the test j has the following elements: (a) the diffusion rate constant η_j which is listed for all soils in Table I; (b) the slope S_j of the CO_2–time curve obtained from fitting a cubic polynomial passing through the origin and the next three data points of each test; and (c) the biological production rate constant μ_j, unknown for the test, but obtained from λ_j after a successive approximation in a manner discussed below. The items needed for a single data point in the test are simply t_i for the sample time and p_i for the total CO_2 produced up to that time, thus having $(t_i, p_i)_j$, $i = 1, 2, \ldots, n$, where n is the total number of data points in the test j.

Now, corresponding to each $(t_i, p_i)_j$ we calculate $(N_i, P_i)_j$, where $N_i = t_i\mu_j$ and $P_i = p_i\eta/S_j$, thus providing $(N_i, P_i)_j$, $i = 1, 2, \ldots, n$, in Fig. 1. Next we calculate $(N_i, Q_i)_j$, using a trial λ_j in the model. From these we calculate the sum of residual squares:

$$r_j = \sum_{i=1}^{n} (Q_i - P_i)^2$$

The latter is calculated for enough trial values of λ_j so that a λ_j vis r_j curve passes through a minimum. The value of λ_j having the smallest residual sum of squares will be assigned to the jth test to complete the transformation of a test as a whole, including its n data points. The transformation, therefore, is essential in our scheme, for through it we are able to calculate the scaler λ.

The functional capacity Q_∞, that is, the value of the ordinate in Fig. 1 corresponding to the equilibrium condition, or the flat part of the curves, is uniquely determined by λ, for all $\lambda < 1$. This value is approached asymptotically and only for tests that are conducted for an infinitely long time, would P_T equal Q_∞. Note that in our tests, T corresponds to t_n of the last data point in a test. When the difference between P_T and Q_∞ is too great due to premature termination of a test, the error in estimating λ would likewise be too excessive and the estimated functional capacity of the microcosm test would be erroneous. It would thus be misleading to unwittingly compare results of those tests that are prematurely terminated with those adequately extended in time for the assessment of the impact of metals. In order to facilitate the proper comparison of tests, a family of theoretical curves constructed with the help of the model to relate the functional capacity Q_∞

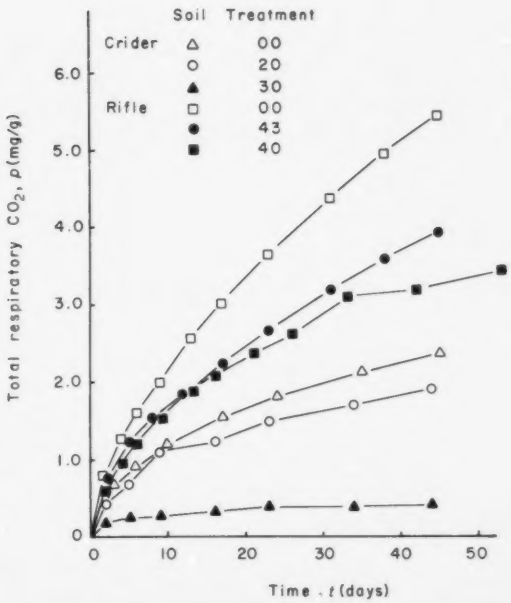

Fig. 2. Typical respiratory microcosm response for control soils (00) and treated with $AgNO_3$ (40, 20, 30), and $CrCl_3$ (43).

of all prematurely terminated tests to the total respiratory values of P_T at the time T of termination. The ratio (P_T/Q_∞) in percent is shown plotted for the family of curves in Fig. 3.

Figure 3 was used to evaluate the adequacy of all test durations in this study. Tables II and III summarize the entire study effort. Table II lists for each of the nine soils and ten metals, the dose level of each treatment, the total duration of a test, the total CO_2 released, and the slope of CO_2–time curve at the origin. Table III provides in addition a two-digit identification code for each test, the calculated λ values and the approach to the functional capacity, R, for that test. The first digit of the identification code refers to the treatment level and the second to the metal compound used. The codes will be used to identify data points when plotted on a graph summarizing interrelationships of functional capacity of various soils.

Henceforth, we will focus attention on test results having $R \geqslant 80\%$. This assures a reasonable accuracy in estimating functional capacity and allows comparisons of nearly similar endpoints in a test. Figure 4 shows one convenient way to present the data using λ, η, and μ. Since Q_∞ is uniquely determined by λ, it needs not be presented. Figure 4 displays numerous physical and biological characteristics of the problem.

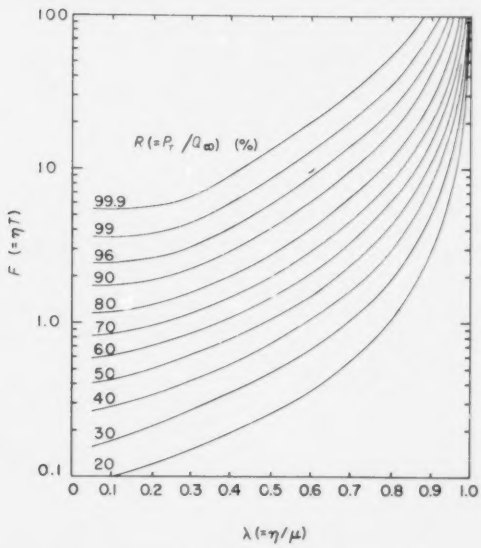

Fig. 3. Approach to theoretical functional capacity for assigned microcosm λ and test duration $F = \eta T$. The system of curve can be used to determine test duration T (day) of new experiments.

The fact that a wide range of soil types has been tested is evident from Table I but it is also apparent from the pattern of curves representing the soils (Fig. 4). Soil conditions typical of high organic content and low resistance to diffusion of CO_2 are represented by the curves in the lower diagonal part of the figure. The lower right side of the figure represents conditions of rapid processing of organic matter (small μ and small η). Along each curve representing a soil type, the respiratory capacity increases with λ as we move downward and to the right. For each point along the curve, there is a fixed production rate constant μ. This means that a soil with fixed physicochemical characteristics may have a biological community that influences respiration differently. The difference could also be due to a relative change in biological response when a chemical compound is added to a soil. Addition of chemical compounds that act as nutrients or stimulators to respiratory function shifts the response on each soil curve downward and to the right. Inhibitory responses have the opposite effects. That is, the points are shifted upward along the trajectory and to the left. Consequently, the system of curves in Fig. 4 may be used as a convenient means of quantifying and interpreting impacts of chemicals on soil respiration.

The broken line in Fig. 4 is the locus of 'control' soil responses. The

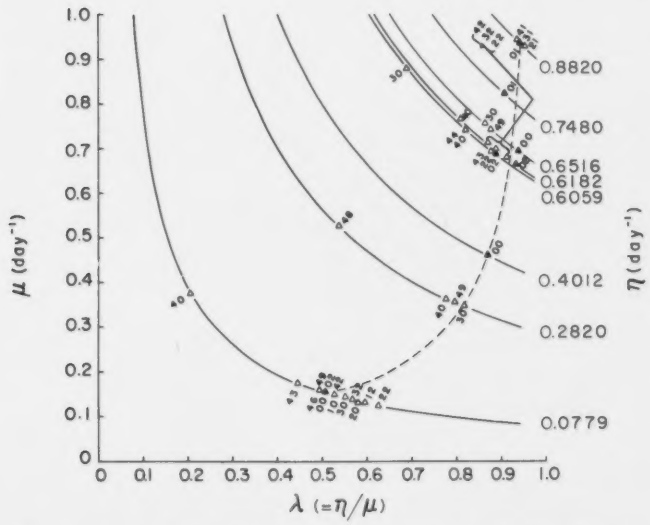

Fig. 4. Effects of various metal compounds on microcosm respiratory functional capacity of various soils. Broken line is the locus of control tests, stimulatory effects fall to the right and inhibitory effects to the left of the line. Two-digit identification codes identify tests as in Table III.

TABLE II

Accumulated respiratory CO_2 (p_T) measured for the duration (T) of the experiments and the slope (S) of the CO_2–time curve at the start of microcosm test

Soil series	Treatment (mmole/kg)	$AgNO_3$			$CdCl_2$			$CdSO_4$			$CrCl_3$			CrO_3		
		T (day)	p_T (mg/g)	S (mg/day)	T (day)	p_T (mg/g)	S (mg/day)	T (day)	p_T (mg/g)	S (mg/day)	T (day)	p_T (mg/g)	S (mg/day)	T (day)	p_T (mg/g)	S (mg/day)
Crider	0.0	45	2.37	0.3259				45	2.37	0.3259	45	2.37	0.3259	45	2.37	0.3259
	0.05	44	2.14	0.3231				45	2.20	0.3031						
	0.5	44	1.90	0.2825				45	2.19	0.3193						
	5.0	44	0.40	0.1478				45	1.67	0.2335						
	50	44	0.20	0.0477				45	1.00	0.1041	45	0.66	0.0970	45	0.45	0.0948
Dayton	0.0				43	1.32	0.1400	43	1.32	0.1400						
	0.5				43	1.22	0.0646									
	5.0				43	0.77	0.0651									
	50				43	0.57	0.0545	43	0.66	0.0482						
Dixonville	0.0				43	3.41	0.3886	43	3.41	0.3886						
	0.5				43	2.87	0.2375									
	5.0				43	2.07	0.1855									
	50				43	1.34	0.0934	43	2.12	0.1454						
Jory	0.0				43	2.66	0.2769	43	2.66	0.2769						
	0.5				43	2.43	0.2173									
	5.0				43	1.71	0.1742									
	50				43	1.11	0.1333	43	1.28	0.1162						

Rifle	0.0	45	5.51	0.5233				45	5.51	0.5233	45	5.51	0.5233	45	5.51	0.5233
	0.05	51	5.92	0.5357				45	5.48	0.4183						
	0.5	51	5.90	0.4751				45	5.44	0.3892						
	5.0	51	5.47	0.4708				45	5.33	0.4300						
	50	51	3.48	0.5176				45	4.46	0.3842	45	3.93	0.4192	45	4.75	0.3525
Sharps-burg	0.0	51	3.38	0.1504				51	3.38	0.1504	51	3.38	0.1904	51	3.38	0.1504
	0.05	50	3.38	0.1568				51	3.31	0.1577						
	0.5	50	3.35	0.1783				51	3.27	0.1493						
	5.0	50	1.57	0.1807				51	2.08	0.1431						
	50	50	1.28	0.1831				51	1.08	0.1194	51	2.06	0.0804	51	1.13	0.0608
Toledo	0.0	47	2.82	0.2491				47	2.82	0.2491	47	2.82	0.2491	47	2.82	0.2491
	0.05	47	2.85	0.2308				47	2.94	0.3201						
	0.5							47	2.74	0.3086						
	5.0							47	2.09	0.2857						
	50	47	0.55	0.1313				47	1.33	0.2180	47	1.46	0.4049	47	1.36	0.2445
Walla Walla	0.0	45	1.03	0.0989				45	1.03	0.0989	45	1.03	0.0989	45	1.03	0.0989
	0.05	45	1.00	0.0900				45	1.16	0.0483						
	0.50	45	0.86	0.0717				45	1.08	0.0572						
	5.0	45	0.40	0.0694				45	0.92	0.0456						
	50	45	0.27	0.0306				45	0.70	0.0350	45	0.48	0.0794	45	0.45	0.0539
Willa-mette	0.0				43	1.44	0.2069									
	0.05				43	1.22	0.0612									
	5.0				43	1.02	0.0574									
	50				43	0.74	0.0554	43	0.80	0.0503						

TABLE II (continued)

Soil series	Treatment (mmole/kg)	$Cd(NO_3)_2$			$CdCl_2$			K_2CrO_4			Na_2CrO_4			$NiSO_4$		
		T (day)	p_T (mg/g)	S (mg/day)	T (day)	p_T (mg/g)	S (mg/day)	T (day)	p_T (mg/g)	S (mg/day)	T (day)	p_T (mg/g)	S (mg/day)	T (day)	p_T (mg/g)	S (mg/day)
Crider	0.0				45	2.37	0.3259				45	2.37	0.3259	45	2.37	0.3259
	0.05															
	0.5															
	5.0															
	50				45	0.78	0.1082				45	0.33	0.0460	44	1.40	0.1296
Dayton	0.0	43	1.32	0.1400												
	0.5															
	5.0															
	50	43	0.54	0.0283												
Dixonville	0.0	43	3.41	0.3886												
	0.5															
	5.0															
	50	43	1.32	0.1094												
Jory	0.0	43	2.66	0.2769												
	0.5															
	5.0															
	50	43	1.12	0.0858												

Rifle	0.0 0.05 0.5 5.0				45	5.51	0.5233	45	5.51	0.5233	45	5.51	0.5233	45	5.51	0.5233
	50				51	4.52	0.4347	45	4.09	0.1867	45	4.35	0.3100	51	4.86	0.4730
Sharps-burg	0.0 0.05 0.5 5.0				51	3.38	0.1504	51	3.38	0.1504	51	3.38	0.1504	51	3.38	0.1504
	50				50	1.80	0.1555	51	1.30	0.0960	51	2.02	0.6105	50	2.93	0.3610
Toledo	0.0 0.05 0.5 5.0				47	2.82	0.2491	47	2.82	0.2491	47	2.82	0.2491	47	2.82	0.2491
	50				47	1.30	0.1961	47	1.17	0.1014	47	1.13	0.1259	47	1.52	0.222
Walla Walla	0.0 0.05 0.50 5.0				45	1.03	0.0989	45	1.03	0.0989	45	1.03	0.0989	45	1.03	0.0989
	50				45	0.41	0.0794	45	0.32	0.0672	45	0.25	0.0522	45	0.66	0.1122
Willa-mette	0.0 0.5 5.0	43	1.44	0.2069												
	50	43	0.71	0.0549												

TABLE III

Rate constants ($\lambda = \eta/\mu$) of microcosm experiments and corresponding approach to theoretical functional capacity ($R = P_T/Q_\infty$); a two-digit code (ID) identifies soil types and chemical treatments

Soil series η (day^{-1})	Treatment (mmole/kg)	(0) $AgNO_3$			(1) $CdCl_2$			(2) $CdSO_4$			(3) $CrCl_3$			(4) CrO_3		
		ID	λ	R (%)	ID	λ	R (%)	ID	λ	R (%)	ID	λ	R (%)	ID	λ	R (%)
Crider (0.6059)	0.0	00	0.8895	84				02	0.8895	84	03	0.8895	84	04	0.8895	84
	0.05	10	0.8787	87				12	0.8881	83						
	0.5	20	0.8815	87				22	0.8812	85						
	5.0	30	0.6900	99				32	0.8858	85						
	50	40	0.8220	95				42	0.9200	73	43	0.8824	85	44	0.8222	95
Dayton (0.6516)	0.0				01	0.9339	68									
	0.5				21	0.9808	28									
	5.0				31	0.9431	61									
	50				41	0.9298	68	42	0.9600	48						
Dixonville (0.4012)	0.0				01	0.8714	74	02	0.8714	74						
	0.5				21	0.9111	60									
	5.0				31	0.9028	64									
	50				41	0.9399	47	42	0.9371	48						
Jory (0.8820)	0.0				01	0.9426	74	02	0.9426	74						
	0.5				21	0.9542	65									
	5.0				31	0.9428	74									
	50				41	0.9382	73	42	0.9543	65						

Rifle	0.0	00	0.5044	86				02	0.5044	86	03	0.5044	86	04	0.5044	86		
(0.0779)	0.05	10	0.5264	87				12	0.5931	76								
	0.5	20	0.5797	82				22	0.6250	72								
	5.0	30	0.5499	84				32	0.5663	79								
	50	40	0.2073	99				42	0.5250	84	43	0.4485	90	44	0.6518	67		
Sharpsburg	0.0	00	0.9736	20				02	0.9736	20	03	0.9736	20	04	0.9736	20		
(0.2820)	0.05	10	0.9686	20				12	0.9643	26								
	0.5	20	0.8486	35				22	0.9695	21								
	5.0	30	0.8139	83				32	0.9038	57								
	50	40	0.7790	85				42	0.8167	81	43	0.9884	08	44	0.9477	37		
Toledo	0.0	00	0.9236	70				02	0.9326	70	03	0.9326	70	04	0.9326	70		
(0.6182)	0.05	10	0.9408	62				12	0.9164	74								
	0.5							22	0.9136	78								
	5.0							32	0.8896	84								
	50	40	0.8122	97				42	0.8713	89	43	0.8705	90	44	0.8666	90		
Walla Walla	0.0	00	0.9395	62				02	0.9295	62	03	0.9395	62	04	0.9395	62		
(0.6516)	0.05	10	0.9426	60				12	0.9952	14								
	0.5	20	0.9464	58				22	0.9734	38								
	5.0	30	0.8660	90				32	0.9753	20								
	50	40	0.9102	79				42	0.9727	39	43	0.8705	90	44	0.8666	90		
Willamette	0.0				01	0.9089	82	02	0.9089	82								
(0.7480)	0.5				21	0.9850	21											
	5.0				31	0.9807	20											
	50				41	0.9612	50	42	0.9741	37								

TABLE III (continued)

Soil series η (day^{-1})	Treatment (mmole/kg)	(5) $Cd(NO_3)_2$			(6) $CuCl_2$			(7) K_2CrO_4			(8) Na_2CrO_4			(9) $NiSO_4$		
		ID	λ	R (%)	ID	λ	R (%)	ID	λ	R (%)	ID	λ	R (%)	ID	λ	R (%)
Crider (0.6059)	0.0				06	0.8895	84				08	0.8895	84	09	0.8895	84
	0.05															
	0.5															
	5.0															
	50				46	0.8970	78				48	0.8863	85	49	0.9314	65
Dayton (0.6516)	0.0	05	0.9339	68												
	0.5															
	5.0															
	50	45	0.9767	32												
Dixonville (0.4012)	0.0	05	0.8714	74												
	0.5															
	5.0															
	50	45	0.9100	60												
Jory (0.8820)	0.0	05	0.9100	60												
	0.5															
	5.0															
	50	45	0.9631	57												
Rifle (0.0779)	0.0				06	0.5044	86	07	0.5044	86	08	0.5044	86	09	0.5044	86
	0.05															
	0.5															
	5.0															
	50				35	0.4983	89	47	0.9225	21	48	0.7431	53	49	0.4968	89

Sharpsburg (0.2820)	0.0				06	0.9736	20	07	0.9736	20	08	0.9736	20	09	0.9736	20
	0.05															
	0.5															
	5.0															
	50				46	0.8697	70	47	0.8988	58	48	0.5390	99	49	0.7973	84
Toledo (0.6182)	0.0				06	0.9326	70	07	0.9326	70	08	0.9326	70	09	0.9326	70
	0.05															
	0.5															
	5.0															
	50				46	0.8606	93	47	0.8357	95	48	0.8411	95	49	0.8807	87
Walla Walla (0.6516)	0.0				06	0.9395	62	07	0.9395	62	08	0.9395	62	09	0.9395	62
	0.05															
	0.5															
	5.0															
	50				46	0.8606	93	47	0.8357	93	48	0.8411	95	49	0.8807	87
Willamette (0.7480)	0.0	05	0.9089	82												
	0.5															
	5.0															
	50	45	0.9575	54												

responses to various chemical compounds can fall to either the right or the left side of this line. Even though only 40% of the data in Table III are displayed they illustrate the trend. For example, the response of untested 'control' soils may be approximated by interpolation with respect to η in this figure. Likewise, the response to an untested level of a chemical can be predicted from previous data as will be discussed later.

Consider the response of Rifle Soil Series ($\eta = 0.0779$ day^{-1}). This is the lowermost curve in Fig. 4. The data points identified by 00, 10, 20, 30, and 40 correspond to five levels of treatment (Table III). The response pattern is: no impact (00); slight stimulation (10); maximum stimulation (20); intermediate stimulation (30); and maximum inhibition (40). A nearly similar reversal pattern is displayed for the effect of $CdSO_4$ (codes 02, 12, 22, 32, and 42) except that all effects are stimulatory even at 50-mmole/kg treatment level. Consequently, all five data points fall to the right hand side of the broken line, indicating a stimulatory effect of the chemical.

Figure 4 displays the relative sensitivity of different soils to a similar treatment. For example, in contrast to the Rifle Soil Series just discussed, the effect of $CdSO_4$ (codes 02, 22, 32, and 42) on Toledo Soil Series ($\eta = 0.6182$ day^{-1}) is totally inhibitory and the response pattern does not display a reversal. A possible explanation for the greater sensitivity of Toledo over Rifle is the greatest organic content and greater buffering capacity of Rifle. There may be other reasons, but the figure displays this characteristic rather well.

APPLICATION

Our results may be used for understanding the respiratory response of soils to metals of untested soil series provided we can estimate the diffusion rate constant η. Consider a soil series having a diffusion rate constant $\eta = 0.5$ day^{-1}. This places the trajectory of its respiratory response between the Dixonville series ($\eta = 0.4012$ day^{-1}) and Crider Series ($\eta = 0.6059$ day^{-1}). The untested soil, therefore, is intermediate in sensitivity to metals relative to these two soils and all impact information can, to the extent data are available, be interpolated to predict response of the untested soil.

Suppose now we wish to conduct a respiratory response test of this soil with no amended metals. Suppose also we were satisfied with a 90% accuracy of approaching the functional capacity. We note again from Fig. 4 that if we plot the trajectory of the untested soil it intersects the broken line, which is the locus of control soils in that figure, at $\lambda = 0.9$. We next enter Fig. 3 with $R = 90\%$ and $\lambda = 0.9$ to obtain $F = \eta T = 44$, from which $T = 44/0.5 = 88$ days. This is the test duration needed to approach 90% of the untested soil's functional capacity.

We can also determine from the two figures that the test duration must be increased when the respiratory process is enhanced (for points falling to the right hand side of the broken line) and the duration can be reduced when the respiratory process is reduced (for points falling to the left hand side of the broken line). The magnitude of change in T can be anticipated roughly from the relative position of a data point on either side of the locus line in Fig. 4.

Better design of experiments aided by the above procedure leads to better understanding of soil response to toxicants. As there are more than 12 000 recognized soil series in the United States alone, any general and convenient scheme that facilitates testing and understanding soil processes should be welcome.

SUMMARY AND CONCLUSION

The time dimension ($N = \mu t$) which is expressed in multiples of respiratory rate constant and μ and the ratio of diffusion to respiratory rate constant ($\lambda = \eta/\mu$) completely predict the dynamic respiratory function ($Q = q\eta/S$) of the soil microcosms. The time dimension may be equally as well represented in multiples of diffusion rate constant ($F = \eta t$). These dimensionless (or unitless) scalers may be regarded as the 'principal components' of the problem. Each scaler combines several of the original variables into one number to reduce the dimensionality of the problem. The scalers contain both biotic and abiotic components. The abiotic components are obtained from the geometry of the experiment and physicochemical properties of the soils. The biotic components (S and μ) relating to the microbial respiration are extracted from the data by calibration of our model which contains these components as parameters. The analysis leads to calculation of a theoretical respiratory capacity which is a function of $\lambda(Q_\infty = 0.4985/(1 - \lambda))$. This is an additional but biologically useful parameter for presenting the data. It can be used to test the adequacy of test duration by comparing it with the measured respiratory capacity P_T. We used this criterion to group our test data for comparability of test information and data accuracy. The data selected in this manner were used to obtain a general parametric graph depicting effects of heavy metal compounds on various soils. Our approach appears to be promising for analyzing microcosm experiments and for predicting the overall response of respiratory capacity.

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GLOSSARY

C	Concentration of CO_2 in soil, a function of t and x (mg/g)
C_0	Initial concentration of CO_2 in soil, assumed constant and uniformly distributed with x (mg/g)
F	Dimensionless time, ηt
G	Biological CO_2 production in soil, a function of t[(mg/g)/day]
G_0	Initial biological CO_2 production [(mg/g)/day]
l	soil depth in microcosm (cm)
N	Dimensionless time, μt
n	Soil porosity (%)
p	Total measured respiratory CO_2 at any time t (mg/g)
p_T	Total measured respiratory CO_2 at any time T (mg/g)
P_T	$= p_T \eta / S$
q	Total theoretical respiratory CO_2 at any time t (mg/g)
q_∞	Total theoretical respiratory CO_2 after a long time (mg/g)
Q	Dimensionless respiratory CO_2 production, $q\eta/S$
Q_∞	Functional capacity, $q_\infty \eta / S$
R	$(P_T/Q_\infty)100(\%)$
S	Slope of total CO_2 — production curve vs. time at $t = 0$ [(mg/g)/day]
T	Duration of experiment (day)
t	Time (day)
x	Space coordinate along soil depth (cm)
α	Diffusivity of CO_2 in soil (cm^2/day); $\alpha \approx 18.7n^2$
λ	Dimensionless rate constant ratio, η/μ (obtained from fitting data with model)
η	Diffusion rate constant (day^{-1}); $\eta = \alpha / l^2$
μ	Biological CO_2 production rate constant (day^{-1})

APPENDIX

Diffusion of CO_2 within a homogeneous layer of soil with internal CO_2 generation $G(t)$ is described:

$$\frac{\partial C}{\partial t} = \alpha \frac{\partial^2 C}{\partial x^2} + G(t) \tag{1}$$

$$G(t) = G_o \exp[(\eta - \mu)t] \tag{2}$$

where $C(x, 0) = C_0$, $C(l, t) = 0$, $G(0) = G_0$ and l is the depth of the soil. The superposition of two solutions for $C(x, t)$ from Carlslaw and Jaeger can be used to accommodate the above initial and boundary conditions: the solution $C_1(x, t)$ with internal heat generation and zero initial concentration (Carlslaw and Jaeger, 1959, p. 131, eq. 9); and the solution $C_2(x, t)$ with constant initial concentration (Carlslaw and Jaeger, 1959, p. 9, eq. 8). The CO_2 flux at the surface is obtained from these solutions by differentiation of the stated equations.

The results are:

$$q = l\eta \left.\frac{\partial C}{\partial x}\right|_{x=l}$$

$$q = q_1 + q_2$$

where

$$q_1 = \eta G_0 \sum_{n=0}^{\infty} \int_0^t \exp[(\eta - \mu)\tau] \exp[-\eta b(t-\tau)]\, \mathrm{d}t$$

$$q_2 = \eta C_0 \sum_{n=0}^{\infty} \exp(-b\eta t)$$

$$b = [(2n+1)\pi/2]^2$$

and

$$\eta = \alpha / l^2$$

The total respiratory CO_2 after time t is:

$$Q = \int_0^t q\, \mathrm{d}t$$

$$Q\eta/S = \sum_{n=0}^{\infty} [\mathrm{I} + \mathrm{II}] \tag{3}$$

I = NUM/DEN, where
NUM = $b \exp[(\lambda - 1)N] + (1 - 1/\lambda) \exp(-b\lambda N) - (1 + b - 1/\lambda)$
DEN = $b(1 - 1/\lambda)(b + 1 - 1/\lambda)$
II = $[1 - \exp(-\lambda b N)]/b$, where
$N = \mu t$
$\lambda = \eta/\mu$

S is the slope of the experimental CO_2 evolution at the origin. We have used it in the following approximation:

$$G_0 \approx lC_0 \approx S \tag{4}$$

In the limit as N tends to infinity, the solution for Q for values of λ less than unity converges to:

$$Q_\infty = \eta/S \int_0^\infty q\, \mathrm{d}t \approx \frac{\mathrm{CONS}}{1 - \lambda} \tag{5}$$

where $0.4985 < \mathrm{CONS} < 0.4933$.

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